Co-Optimization of
Fuels & Engines

Multimode Lean SI: Experiments and Simulation

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FY17 Vehicle Technologies Office
Annual Merit Review

better fuels | better vehicles | sooner

Project ID: FT055

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

VTO Management: Gurpreet Singh, Kevin Stork, Leo Breton, and Mike Weismiller

Overview

These light-duty SI engine research tasks support both :

- Near-term Co-Optima fuel-economy targets for conventional boosted SI.
- Longer-term development of fuels for advanced highly efficient SI combustion.

Tasks / Budget

- E.1.1.3: Advanced Light-Duty SI Engine Fuels Research: Multiple Optical Diagnostics of Well-mixed and Stratified Operation
  (SNL, Sjöberg - $652k, FY16 & 17)
- E.1.1.4: Advanced Light-Duty SI Engine Fuels Research: Knock Limits and Imaging of Turbulent Flame Development
  (SNL, Sjöberg - $300k, FY16 & 17)
- G.2.1: Sandia DISI Engine Simulations
  (ANL, Som - $255k, FY16 & 17)

Timeline

- Project start date: 10/1/2016
- Project end date:* 9/30/2018
- Percent complete: 56%

* Start and end dates refer to three-year life cycle of DOE lab-call projects. Co-Optima is expected to extend past the end of FY18.

Partners / Collaborators

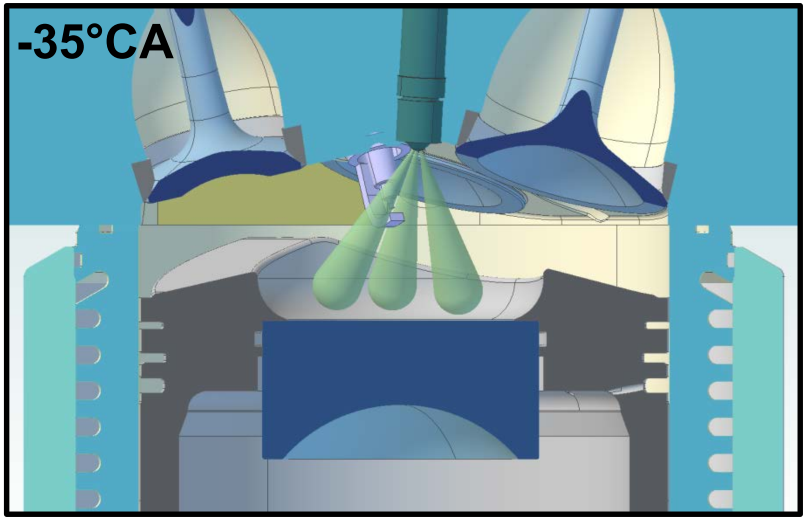
- 15 Industry partners in the AEC MOU.
- General Motors - Hardware.
- Toyota – Funds-in knock project (not VT).
- TU Darmstadt – Optical diagnostics.
  - C. Ding as visiting Ph.D. student.
- X. He (long-term visitor from BIT.)
- D. Vuilleumier (SNL post-doc).
- N. Van Dam (ANL post-doc)
- W. Zeng (former SNL post-doc, now GM).
- D.L. Reuss (formerly at GM).
- ANL (R. Scarcelli *et al.*) – RANS CFD.
- LLNL (W. Pitz *et al.*) – Chemical kinetics.
- Transient Plasma Systems Inc.

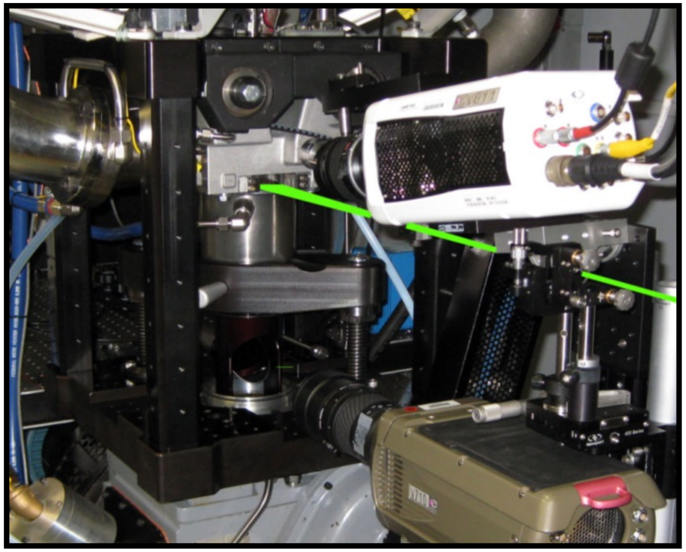
Approach

- Combine metal- and optical-engine experiments and modeling to develop a broad understanding of the impact of fuel properties on DISI combustion processes.
  - Utilize Co-Optima Core fuels with common RON = 98 specification. (E30, High-Aromatics, Alkylate, High-Olefin, & High-Cycloalkane.)
  - Examine promising blendstocks (*e.g.* iso-butanol, di-isobutylene, 2-butanol) in mid-level RON98 surrogate blends.
- First, conduct performance testing with all-metal engine over wide ranges of conditions.
  - Speed, load, intake pressure, EGR, and stratification level.
  - For conventional stoichiometric operation: Determine knock limits. Compare fuels within octane-index framework and assess validity of Central Fuel [Properties] Hypothesis.
  - For non-conventional SI operation (stratified and ultra-lean): Identify critical combinations of operating conditions and fuels.
  - Relate exhaust smoke emissions to Particulate Matter Index (PMI).
- Second, apply a combination of optical and conventional diagnostics to develop the understanding needed to mitigate barriers.
  - Include full spectrum of phenomena; from intake flows, fuel injection, fuel-air mixing, spark development and ignition, to flame deflagration and end-gas autoignition.
- Enhance understanding through concurrent modeling efforts.
  - CFD modeling with fuel-properties variations and global sensitivity analysis.
  - Chemical-kinetics modeling of end-gas autoignition reactivity.
- Utilize experimental and modeling results to validate and improve Merit Functions.

Approach – Engine / Diagnostics

- Drop-down single-cylinder engine. Bore = 86 mm, Stroke = 95 mm, 0.55 liter, CR = 12.
- Piston bowl and closely located spark and injector.
  - Highly relevant for stratified operation. 8-hole injector with 60° included angle.
- Identical geometry for all-metal and optical configurations
  - Minimal discrepancy between performance & emissions testing and optical tests.





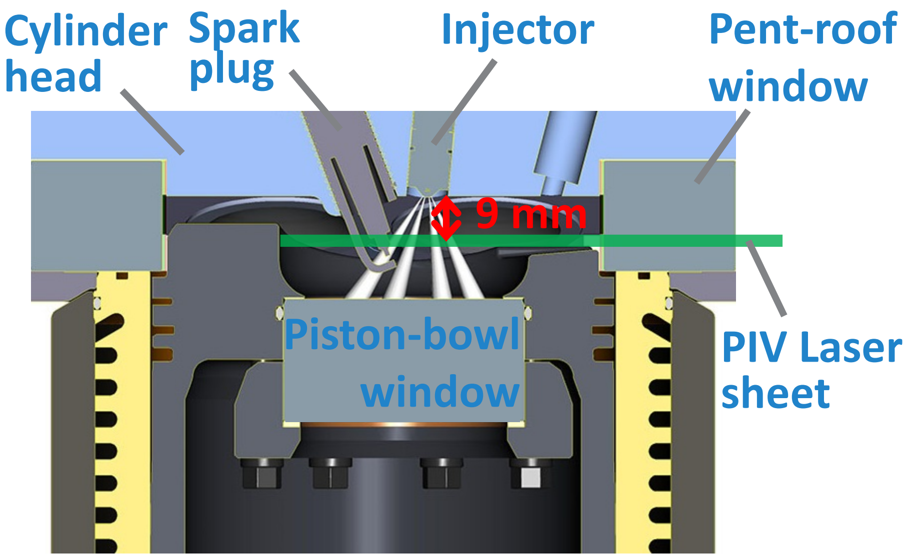
- Apply a range of high-speed optical diagnostics:
  - PIV – Flows, Mie - Liquid Spray, RIM - Wall Wetting, IR - Fuel Vapor. Plasma & flame imaging.
- Apply advanced ignition when it increases relevance of the fuels research.

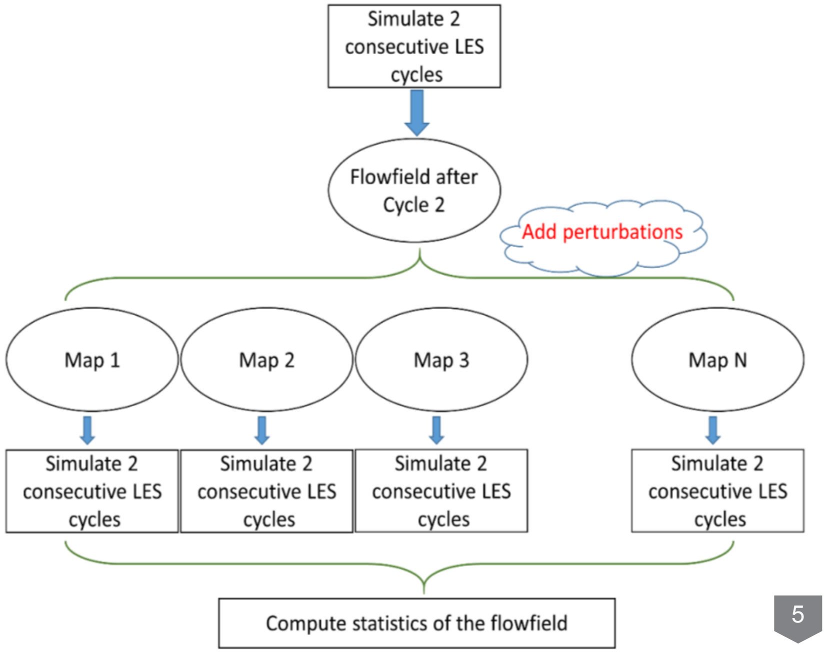
Approach – CFD Modeling

- Optical access allows validation of flow and quantities beyond pressure.
  - Adds confidence when applying models to other engine configurations.
- CFD of this engine will focus on fuel property effects.

Two CFD-simulation approaches:

- Multi-cycle LES, with higher fidelity.
  - More detailed investigations, including CCV.
  - Parallel cycle approach* for faster turnaround.
- RANS
  - Lower computational overhead.
  - Used for investigations of broad trends and/or where many simulations are required, *e.g.* sensitivity analysis.

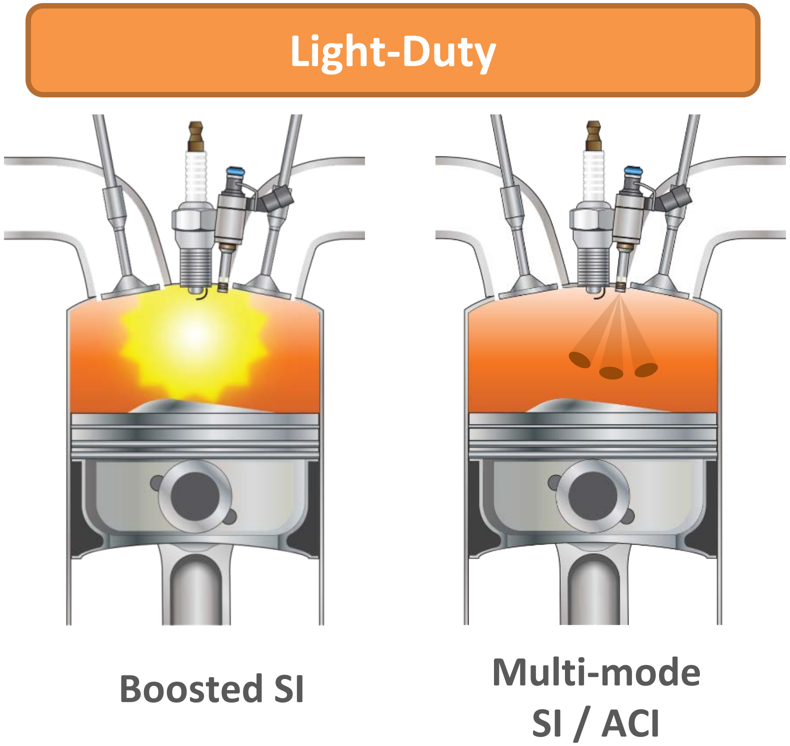




*Ameen, M. M., Yang, X., Kuo, T. W., & Som, S. (2016). Parallel methodology to capture cyclic variability in motored engines. International Journal of Engine Research, DOI:10.1177/1468087416662544

Relevance

- Increased fuel economy requires engines with higher thermal efficiency, while complying with stringent exhaust requirements for clean air.
- Hence, these **light-duty** engine fuels studies are focused on:
  - Thermal efficiency as controlled by knock limits for **boosted stoichiometric SI operation.**
  - Emissions mitigation for more efficient **stratified-charge SI operation**.
  - Efficiency gains for **ultra-lean well-mixed SI operation** that utilizes mixed-mode combustion (with transition from deflagration to autoignition).
- Co-Optima:
  - Strengthen or challenge Central Fuel Hypothesis.
  - Refine existing merit function for stoichiometric SI.
  - Develop new merit functions for advanced combustion modes.
  - Tier 3 testing of promising fuel candidates.
- Broader engine-combustion science:
  - Inform industry of fuel effects on advanced combustion modes.
    - Pre-competitive with TRL = 2 – 4.
  - Advance optical-engine diagnostics.
  - Advance CFD models and methodology.



Milestones – FY16 -17

✓ • **June 2016, SNL:** Analyze effects of electrode configuration on multiple-pulse transient plasma ignition.

✓ • **Sept 2016, SNL:** Quantify statistically flame-spread variability for boosted stratified-charge SI operation using E30 and gasoline.

✓ • **Dec 2016, SNL:** Provide validated GT-Power model of DISI engine to the Co-Optima Toolkit Development Team.

✓ • **Dec 2016, SNL:** Transfer flow, flame, and combustion validation data for well-mixed stoichiometric and lean E30 operation to the Co-Optima Toolkit Development Team.

Data are available • **March 2017, SNL:** Provide fuel-efficiency and exhaust-emissions data for SI engine operation with both a baseline AKI87 and a RON98 gasoline to the Co-Optima ASSERT Team.

✓ • **March 2017, SNL:** Quantify differences of post-injection flow speeds near spark plug for stratified operation with single and double injections.

✓ • **March 2017, ANL:** Sensitivities to fuel properties at validation points (Sandia DISI engine, stoichiometric operation).

✓ • **June 2017, SNL:** Finalize a comparative study on knock limits for three Co-Optima core fuels.

✓ • **June 2017, SNL:** Finish an initial investigation on the effect of spark-plug location on lean stability limits.

• **Sept 2017, SNL:** Provide quantified turbulent flame development rates for well-mixed stoichiometric, lean and dilute SI engine combustion, using Co-Optima core fuels.

✓ • **Sept 2017, ANL:** Sensitivities to fuel properties at validation points (Sandia DISI engine, stratified-charge operation).

• **Sept 2017, SNL:** Determine if a new biofuel component blended to gasoline changes the dominant soot-production pathway for stratified-charge SI combustion.

Technical Accomplishments

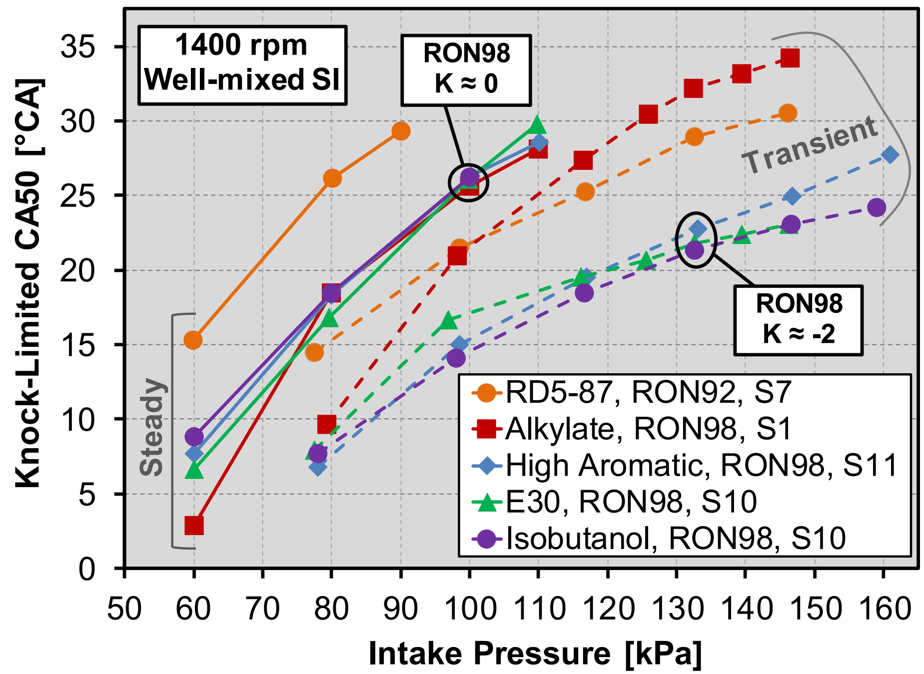
- Measured stoichiometric knock limits for five fuels, both steady-state and transient.
  - Related knock limits to RON, MON, and octane sensitivity within the Octane-Index framework.
  - Demonstrated the role of low-temperature heat release for poor performance associated with low octane sensitivity.
- Shown when PMI predicts smoke emissions, and when it does not.
- Identified how soot-production pathways change with fuel type and operating conditions for stratified-charge SI operation.
- Developed semi-quantitative wall-wetting diagnostics based on refractive index matching (RIM).
- Examined how high HoV of E30 leads to increased wall wetting and pool fires.
- Completed a study on the combined effect of intake flow and spark-plug location on lean-stability limits.
  - Demonstrated optical diagnostics of deflagration-to-autoignition transition.
- Validated in-cylinder flow using LES-based CFD for three operating points.
- Performed fuel-properties combustion study using RANS-based CFD modeling.
  - Used Global Sensitivity Analysis (GSA) to identify most influential fuel properties.
- Contributed to a refined Merit Function.
  - RON, S, HoV, S_L and PMI terms.

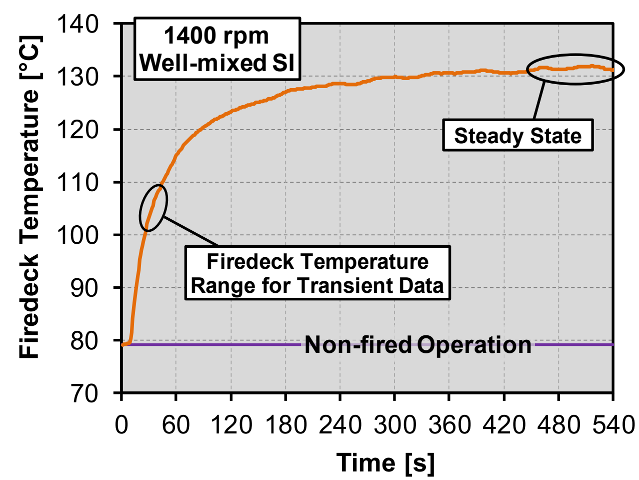
Stoichiometric Knock Limits for 5 Fuels

- Intake-pressure sweeps reveal how fuels respond to load and engine conditions.
- RON and MON are determined for steady-state conditions.
- Actual vehicle operation is usually not steady-state.
  - Acquire load-transient data as well.
  - Thermally analogous to a temporary (≈20s) increase of load.
- RON98 fuels overlap for P_{in} = 100 kPa.
  - Conditions are best characterized by K = 0.
- For boosted transient operation, K is highly negative.
  - Here, high-S fuels show great benefits.

- Generally, KL-CA50 rank order are explained well by RON and S.
  - Within OI framework.
- Supports Central Fuel Hypothesis.

- Iso-butanol performs slightly better than RON & S indicate.

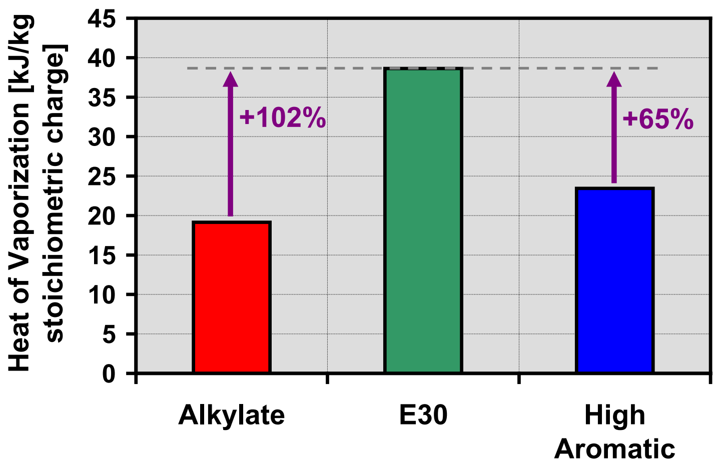


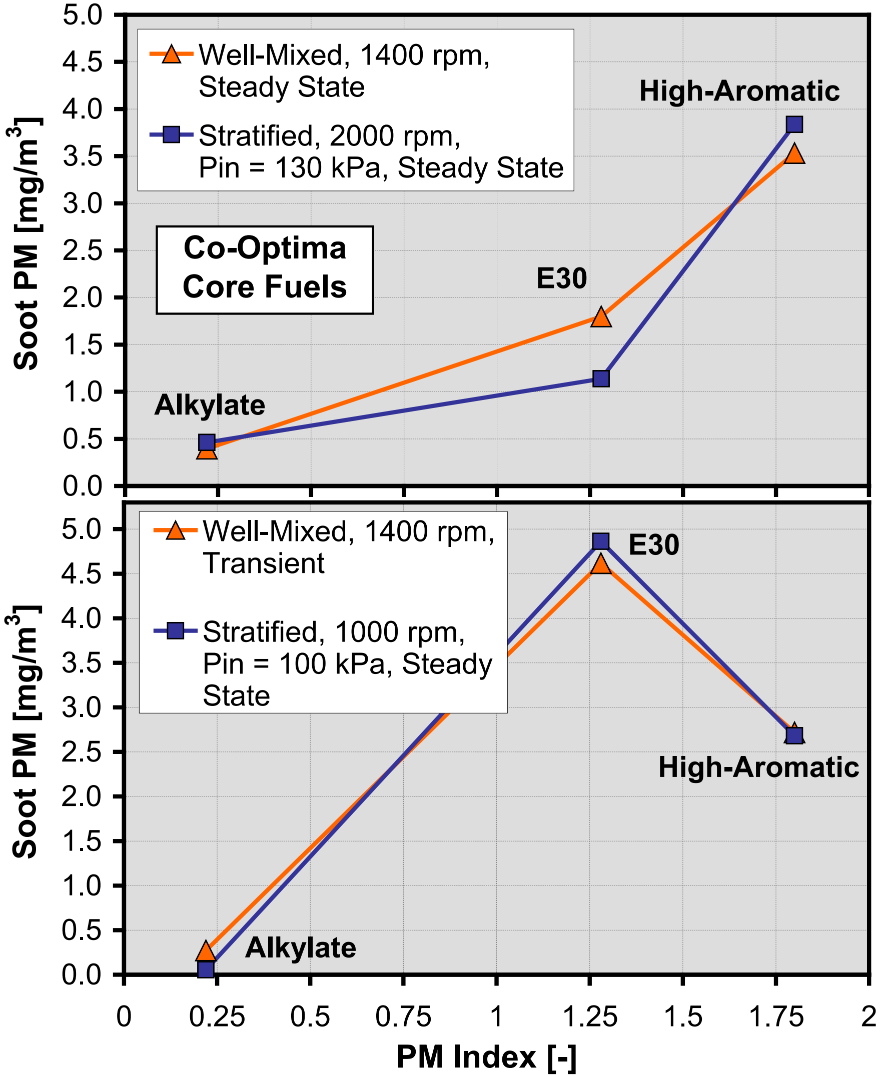


Assessment of PMI for Various Modes of Operation

- Steady-state well-mixed stoichiometric PM scales as per original formulation of Merit Function.
  - x3 for each PMI unit increase.
- Trend of boosted stratified-charge operation is in general agreement.

- PM of E30 is not consistent with PMI for transient stoichiometric, nor for non-boosted stratified.
  - Wall-wetting issues due to high charge-specific HoV of E30.



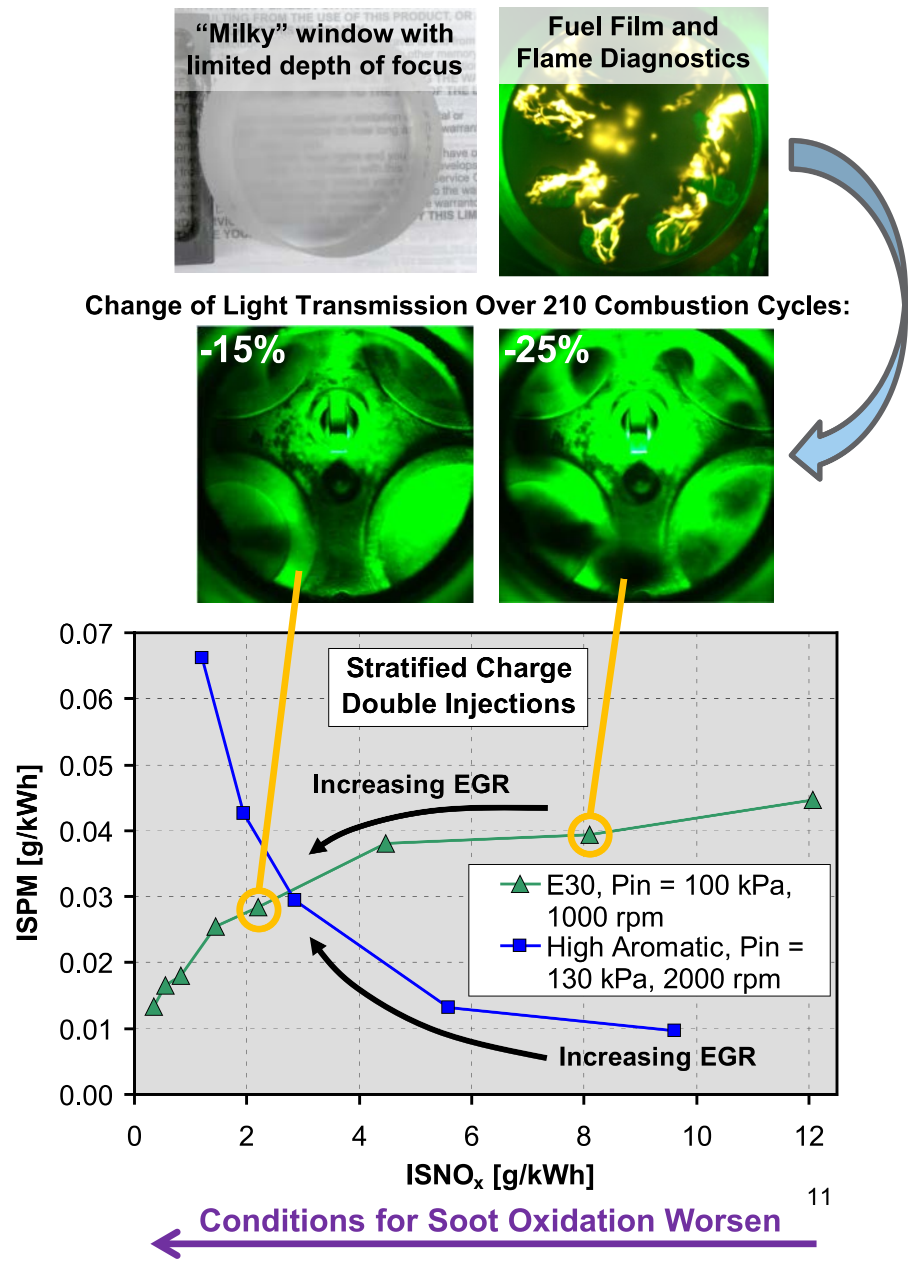


Soot-Production Pathways for Stratified Operation

- Low NO_x is required to reduce aftertreatment burden for efficient stratified-charge SI oper.
  - Mandates the use of EGR.
- Response of engine-out soot to EGR varies greatly with fuel and operating conditions.
- Engine-out soot = (Soot formed) – (soot oxidized)
- Soot oxidation will be impeded by EGR.
- Explains traditional NO_x / PM trade-off.

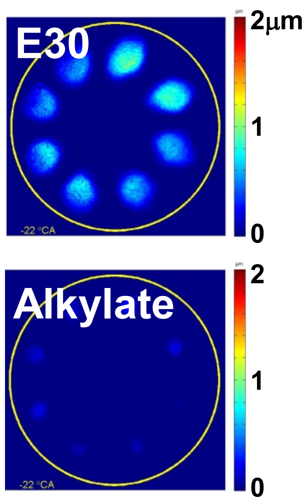
- Bulk-gas soot formation for boosted operation at 2000 rpm. (See AMR 2016.)
  - Here, PMI is predictive.
- For non-boosted operation with E30, soot formation is controlled by intensity of pool fires.
  - PMI is not predictive.

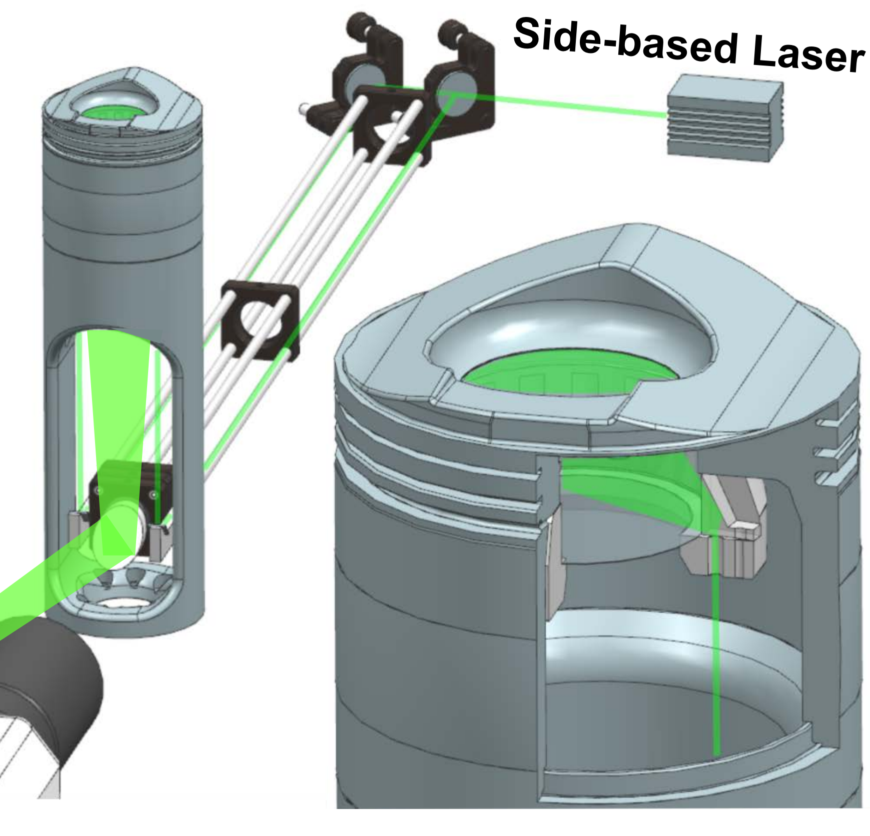
- Increased pool-fire activity for higher $[O_2]$ is evidenced by soot deposits.
- “Milky”-window technique allows determining wall-wetting and near-wall flames.
- Parametric fuel studies are ongoing.



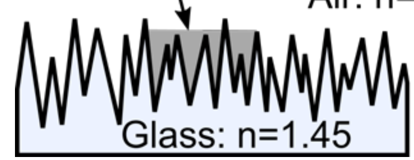
Development of Wall-Wetting and Pool-Fire Diagnostics

- Literature on RIM technique was unclear on how to achieve most effective setup ⇒ Examined the use of two types of light sources (laser vs. LED), and illumination angle (front vs. side).
- Front illumination is easier to implement, and provides quantification of fuel-film area.
- Side illumination provides both area quantification, and semi-quantitative thickness.
- Type of light source does not matter (coherent laser or LED, pulsed or CW.)

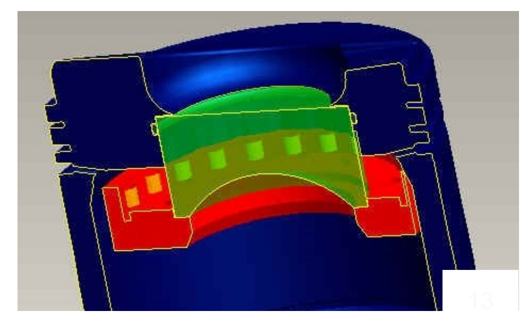




- Window surface roughness is very important.
  - R_a = 7μm works well for thickness measurements.



Side-based LED



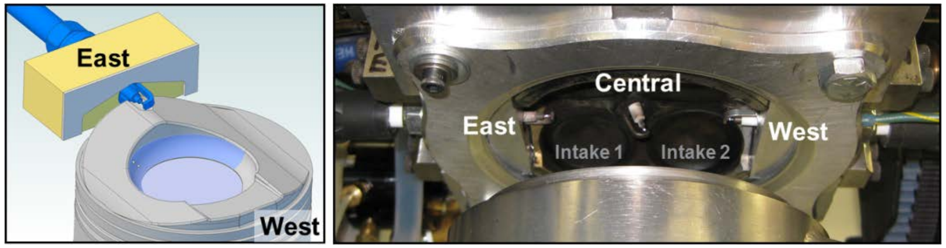
Illustrations by C. Ding, TU Darmstadt and X. He, Beijing Institute of Technology.

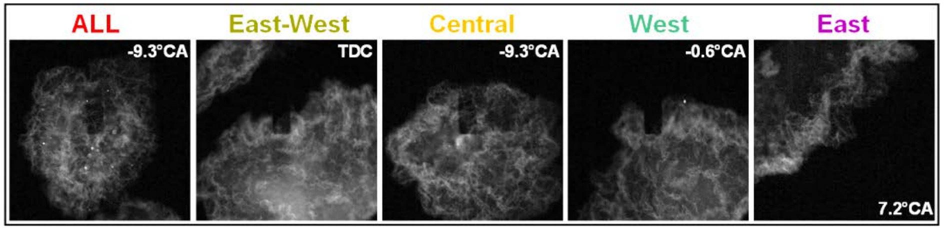
Effect of Intake Flow and Spark Location on Lean Operation

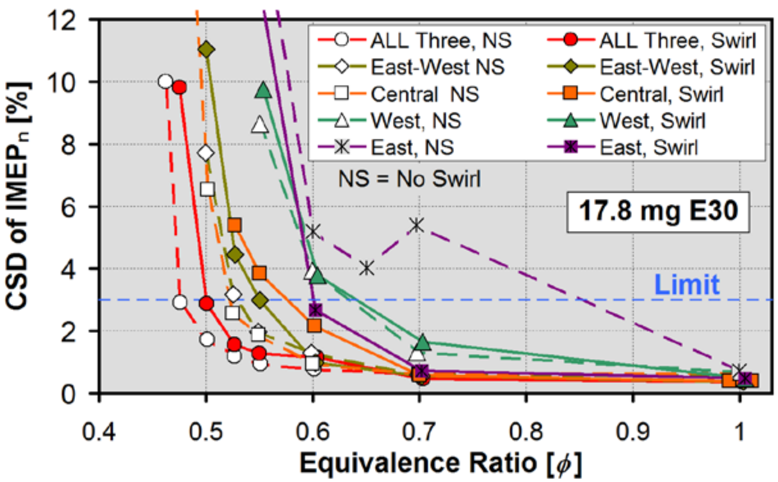
- Mixed-mode combustion is one option for maintaining short burn duration for ultra-lean operation.
- Poorly understood, especially fuel effects on flame-to-autoignition transition.

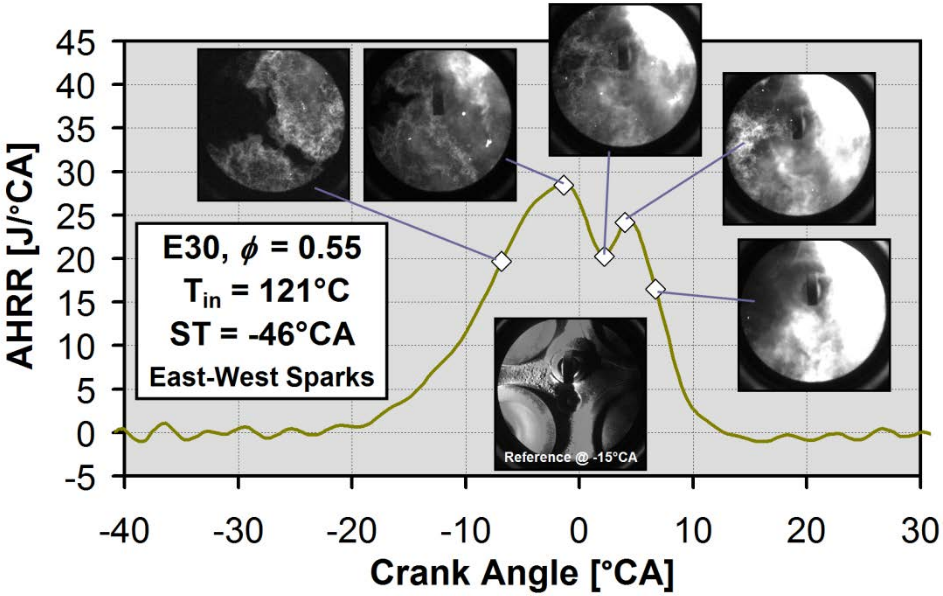
> - Several flow/spark scenarios enable stable ultra-lean oper. w/ +20% η_{th}.
>   - "Tumble only" generally speeds up flame development.

- H-S imaging of transition is feasible for East-West spark scenario.





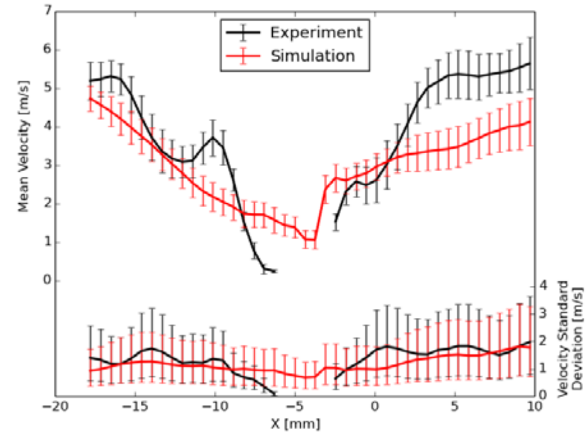




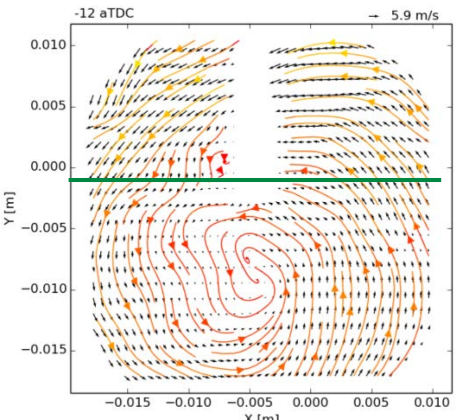
LES Flow Validation for Stoichiometric Operation

- Intake and compression with early fuel Injection.
- Throttled, well-mixed SI operation.
- Averages over 30-35 engine cycles.
- Examples shown near spark timing.

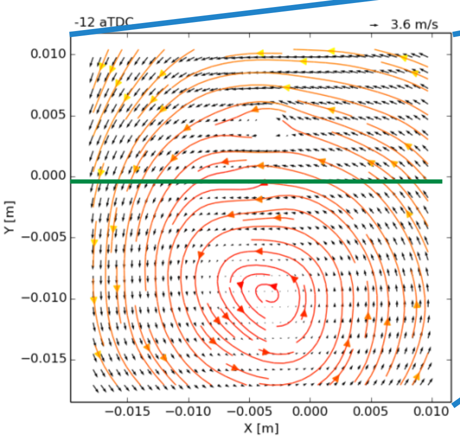
- **Flow pattern generally reproduced.**
- Simulations more symmetric across spark plug gap.
- Pressures well-matched, slightly lower sim peak.

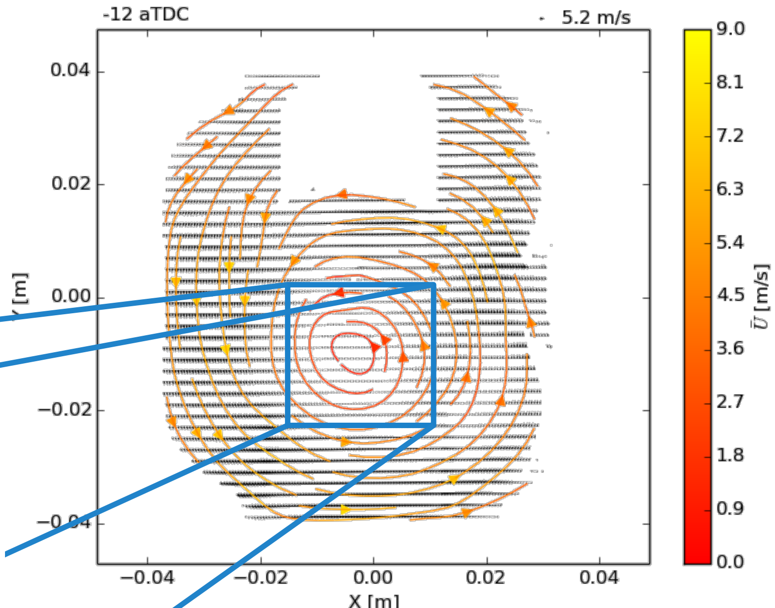


Particle Image Velocimetry

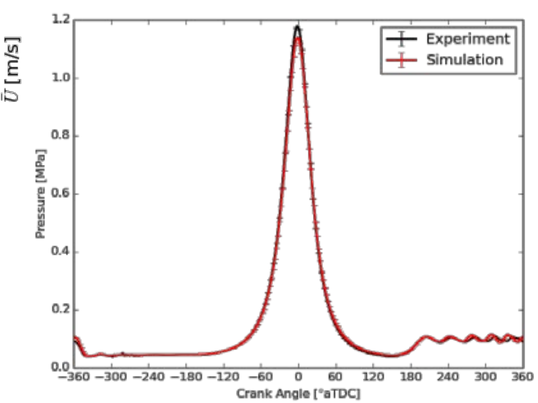


Simulation (PIV Window)





Simulation (Full-Plane)

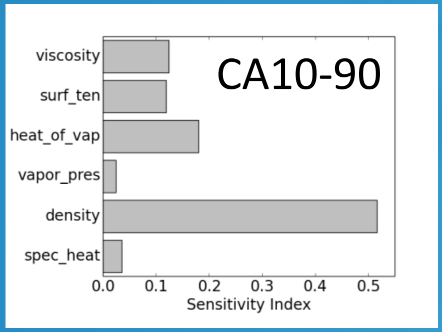


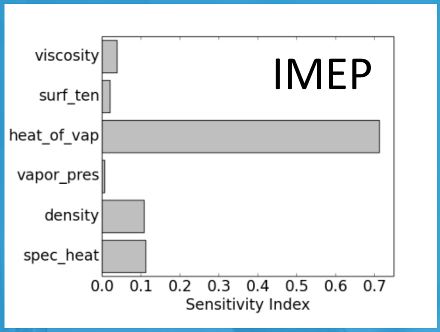
Accomplishments
Effect of Fuel Properties for RANS Model using GSA Methodology

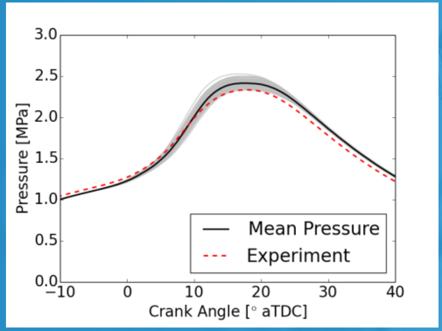
- Fuel properties of an E30 fuel varied in a Monte-Carlo fashion.
  - 6 varied ±10%: Viscosity; Surface Tension; Heat of Vaporization; Vapor Pressure; Density; Specific Heat.
- Global Sensitivity Analysis shows which parameters have the largest impact.
  - $SI_i \equiv \frac{\mathrm{Var}_{X_i}\left(\mathrm{E}_{X_{\sim i}}(y|X_i)\right)}{\mathrm{Var}(y)}$
  - $\equiv \frac{Variance\ in\ y\ due\ to\ input\ X_i}{Total\ target\ y\ variance}$
- Burn duration most strongly influenced by density, but effect is relatively weak.
- A linear fit shows the general direction.
  - $y(x) = \alpha_0 + \sum_i^n \alpha_i x_i$
  - Also gives an approximate measure in change of target per percent-change in an input variable

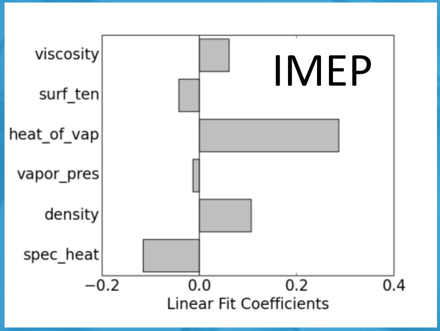
- Heat of vaporization dominates over other variables for IMEP.
- Inform Merit Function development effort.

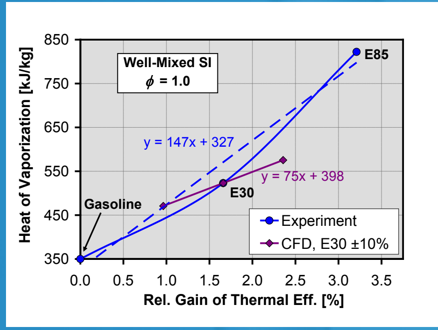
- This analysis technique is applicable to other engine platforms.
- Currently being applied to Scott Sluder's engine at ORNL.

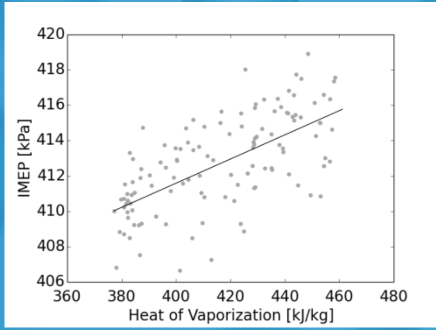






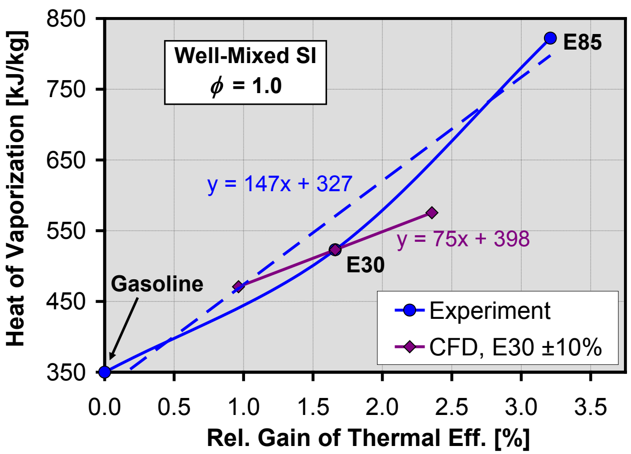


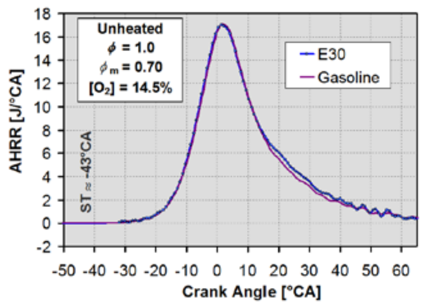


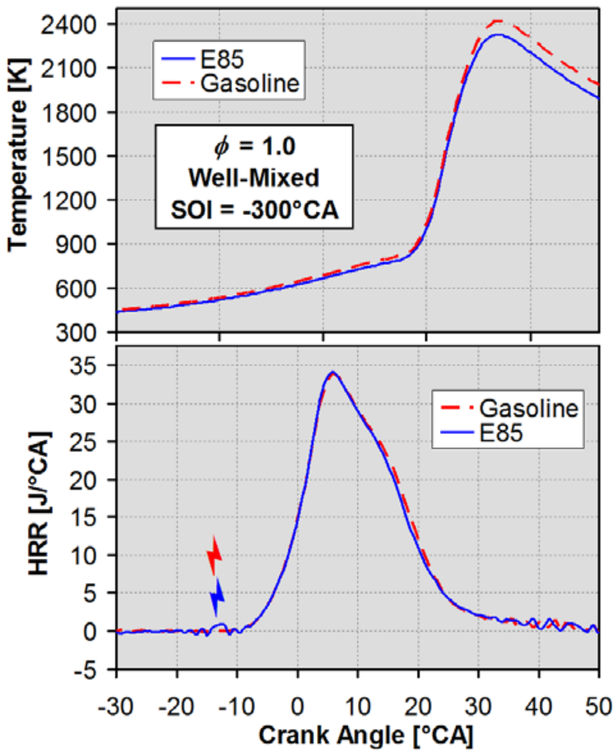


Merit Function Refinement - HoV Benefit

- Smoke vs. PMI trends discussed above. (RON & S benefits shown in extra slides.)
- Gasoline-ethanol blends are uniquely qualified for assessing direct gain of higher HoV on η_{th} for non-knock limited SI operation.
  - Inherent higher flame speed of ethanol compensates perfectly for lower charge temp. with higher HoV.
  - Examples for stoichiometric dilute and non-dilute operation.





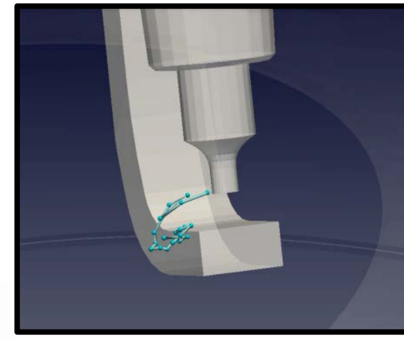


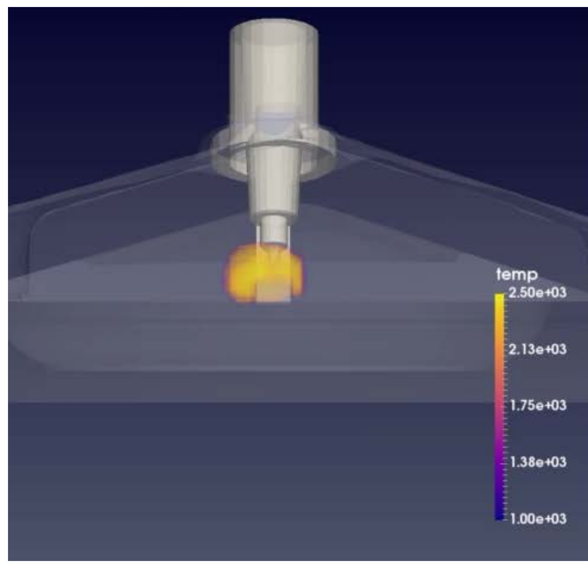
- Available data support HoV benefits of originally proposed Merit Function.
- CFD results indicate that incremental benefit per [kJ/kg] of HoV is higher than what is realized across full E0 – E85 range.
  - Justifies further examination.

Collaborations

- Collaborating with Scarcelli *et al.* at ANL on ignition models for CFD.

- RANS-CFD validated well against experimental flow field.
- Early flame kernel growth for $\phi = 1$ compares well against ensemble-averaged flame luminosity.



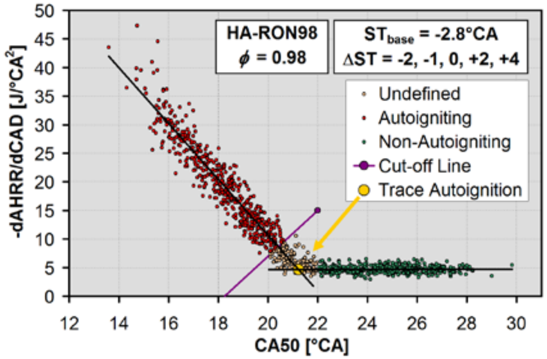


- Next steps include ultra-lean SI operation and advanced ignition.
- Isaac Ekoto will experimentally evaluate fuel-specific advanced-ignition chemical and physical mechanisms at SNL.

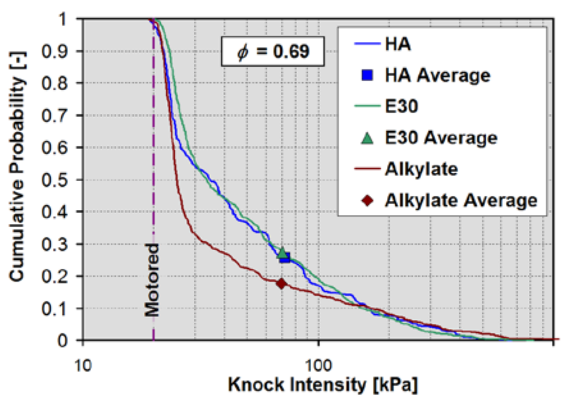
Note: Any proposed future work is subject to change based on funding levels.

Collaborations (2)

- Funds-in Project with Toyota.
- Developed HRR-based method for well-defined conditions corresponding to "trace" end-gas autoignition.

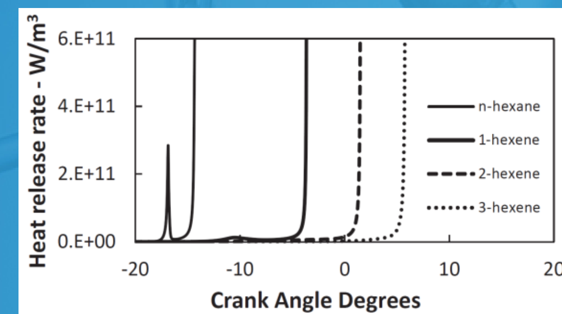


- Valuable diagnostics tool. E.g. for determining factors that cause differences in knock statistics.



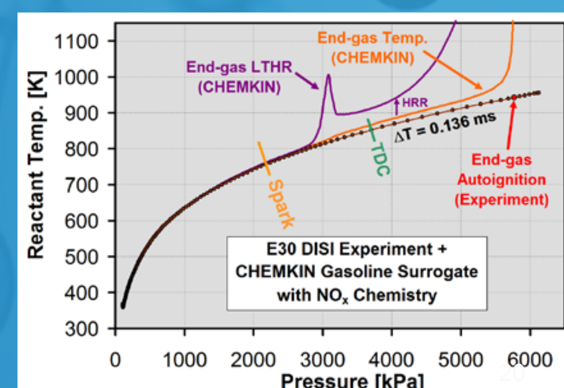
- Alkylate fuel with low S shows wider acoustic knock distribution.

- Collaborating with Pitz, Westbrook & Mehl on the role of fuel molecular class and structure for octane sensitivity.
  - Used RON- and MON-like DISI-engine data as input to CHEMKIN-PRO.
- Olefins: Location of double-bond strongly affects early autoignition reactions.



- Examining the role of trace species (*e.g.* NO_x) on autoignition reactions.

– Enhancing fidelity of reaction mechanisms.



Responses to Previous Year Reviewers' Comments

- Feedback on 'Co-Optima Overview': "…the optical single cylinder engine at Sandia National Laboratories (SNL) is an excellent tool for helping with the development and validation of computational models but that engine is not representative of the Thrust I production engine technologies. The reviewer said that the use of the optical engine to validate computational models may lead to validation of combustion regimes, which would not be encountered in Thrust I production technology."
- Answer: For knock work, the Sandia DISI engine is primarily used to validate flow and spray sub-models, and the CFD model are currently being applied to an engine at ORNL, which has been deemed more relevant for boosted SI work.

- Feedback on 'Fuel Properties and Thrust I Engine Research': "Having Thrust I and Thrust II fuels be the same is an incredible opportunity to further the main goal of Co-Optima vision of "Better fuels and better vehicles sooner.", also "…the use of an Octane Index (OI) as a means to evaluate fuel properties simultaneously suitable for both Thrust I and Thrust II engines is encouraged."
- Answer: We agree that using the same fuel for both boosted SI and emerging advanced SI combustion is an opportunity that warrants examination. Along the lines suggested, we are indeed examining the use of these Thrust I fuels for advanced lean/dilute combustion modes, including the assessment of autoignition reactivity within the OI framework.

- "…the reviewer remarked that the Co-Optima program should verify that high RON and high sensitivity fuels do indeed substantially increase engine and vehicle fuel efficiency . The reviewer commented that this should be done quickly and with minimal research, as this ground has been plowed numerous times by many studies, and the answer is generally well-known and accepted."
- Answer: This stoichiometric boosted SI knock work makes up a relatively small portion of these tasks, and will be concluded by the end of FY18.

- Feedback on 'Thrust II Engine Research, Sprays Research, and Emissions Control Research': "The reviewer questioned if particulate matter index (PMI) translated from Thrust I to Thrust II. "
- Answer: This is a very interesting question. As shown in this presentation, the experiments to date indicate that PMI can predict soot emissions for stratified-charge SI operation as long as the soot production is not dominated by wall wetting.

Proposed Future Research FY17 - 18

Experimental work at SNL (Sjöberg)

- Finish boosted stoichiometric knock work (Tier 3 fuel assessment).
- Use Co-Optima core fuels and new promising fuel blends to map out autoignition limits for lean and EGR-diluted SI operation with well-mixed charge.
  - Determine relevance of RON, MON and the OI framework for lean or dilute SI engine operation.
- Optically investigate end-gas autoignition for lean well-mixed mixed-mode SI combustion, to determine how different fuels affect flame structure and peak HRR.
- Optically investigate fuel effects on transient plasma ignition used to stabilize ultra-lean mixed-mode SI operation. (SNL PI: Ekoto.)
- Investigate fuel effects on efficient stratified-charge SI operation, with a focus on pathways for soot emissions (pool-fires due to wall-wetting vs. bulk gas).
  - Initiate hardware upgrades: Higher injection pressure and better PM instruments.

CFD work at ANL (Som)

- Complete multi-cycle LES simulations with combustion.
- Investigate additional operating conditions.
  - More unstable conditions closer to knocking limits.
  - Advanced combustion strategies.
- Examine the large SI parameters to help analyze reasons for the strong dependencies.
- Analyze input parameter interaction effects.
  - Include fuel chemical effects.

Note: Any proposed future work is subject to change based on funding levels.

Summary

- These tasks are contributing strongly to both the Co-Optima project and to the science of fuel/combustion interactions for advanced SI engine combustion.
- Experiments combined with CFD modeling contribute to a refined Merit Function.

- In-cylinder flows validated well against experiments for LES-based CFD.
- Global Sensitivity Analysis (GSA) of a RANS-based CFD model indicates that HoV is most influential on IMEP for a non-knock-limited operating point.
- Mapped out stoichiometric knock limits for five fuels, both steady-state and transient.
  - Generally, rank order of fuels is consistent with RON, MON, and octane sensitivity within the octane-index framework. Strengthens Central Fuel Hypothesis.
- For this DISI engine, PMI predicts well exhaust soot for fully warmed-up steady-state.
  - Does not work for E30 under colder transient operation, nor for stratified with wall-wetting.
- For stratified-charge combustion, wall wetting and pool fires become a dominating soot-production pathway when E30 fuel is used for non-boosted operation.
- Wall-wetting diagnostics based on refractive index matching (RIM) works well both with LED- and laser-based illumination.
  - “Milky” window also allows determination of near-wall flames, *aka* pool fires.
- Intake flow without swirl generally provides faster inflammation and more stable ultra-lean well-mixed SI operation. Rel. η_{th} gain = +20 % with mixed-mode combustion.
  - Using two side-mounted spark plugs, the transition from deflagration to autoignition can be imaged well for research purposes.

Acknowledgement

- The experimental work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
- The CFD work was done by UChicago Argonne, LLC, Operator of Argonne National Laboratory (Argonne). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DEAC02-06CH11357.

Technical Backup Slides

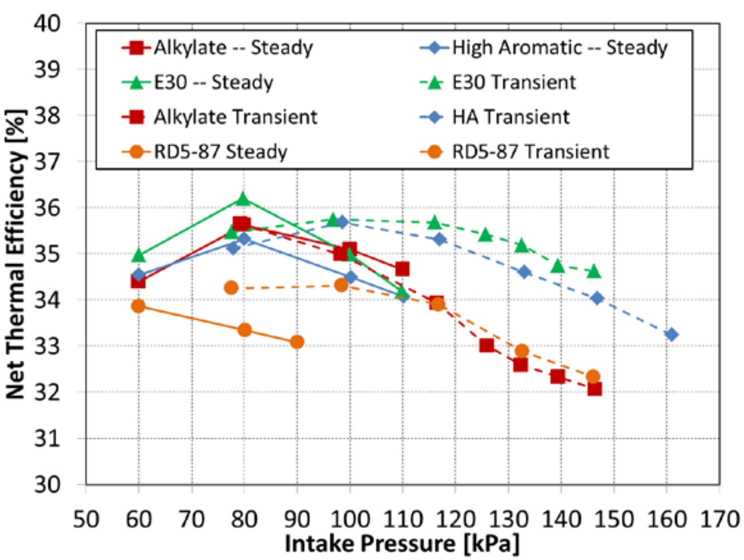
Merit Function Refinement - RON and S Benefits

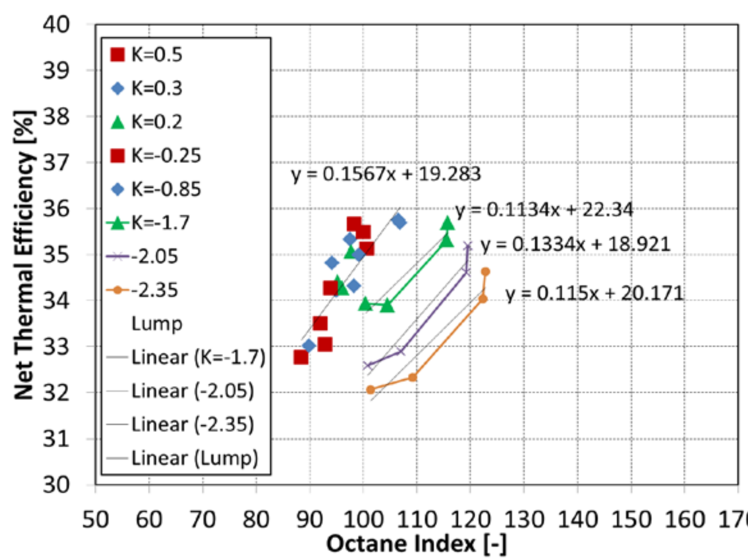
- Analyzed data for four fuels within OI framework to assess RON and S terms of originally proposed Merit Function for knock-limited SI operation.

- Measured increase of η_{th} is somewhat lower than predicted by Merit Function.

- However, the Merit Function accounts for both increased CR, as well as additional downsizing.

K Range	Relative Thermal Efficiency Gain (%) per Octane Index Unit (-)	Relative Thermal Efficiency Gain (%) per Octane Index Unit (-) Multiplied by 1.1 (for downsizing/boosting effects)	Merit Function Relative Efficiency Gain per OI Unit
K = -0.85 : 0.5	0.48	0.53	0.625
K = -1.7	0.33	0.37	
K = -2.05	0.41	0.45	
K = -2.35	0.36	0.39	
Average	0.39	0.43	



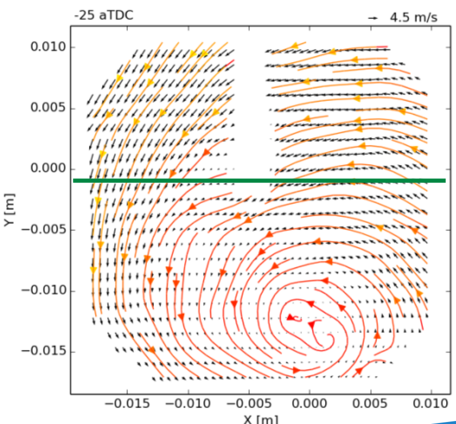


LES Flow Validation – Intake and Compression for Stratified-Charge Operation

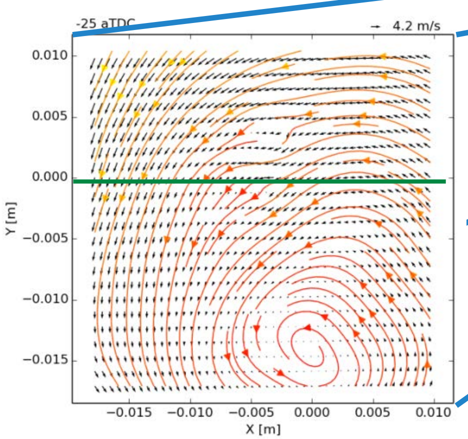
- Un-throttled, stratified operation.
- Averages over 16 experiment, 30 simulation engine cycles.
- Data shown near nominal spark timing.

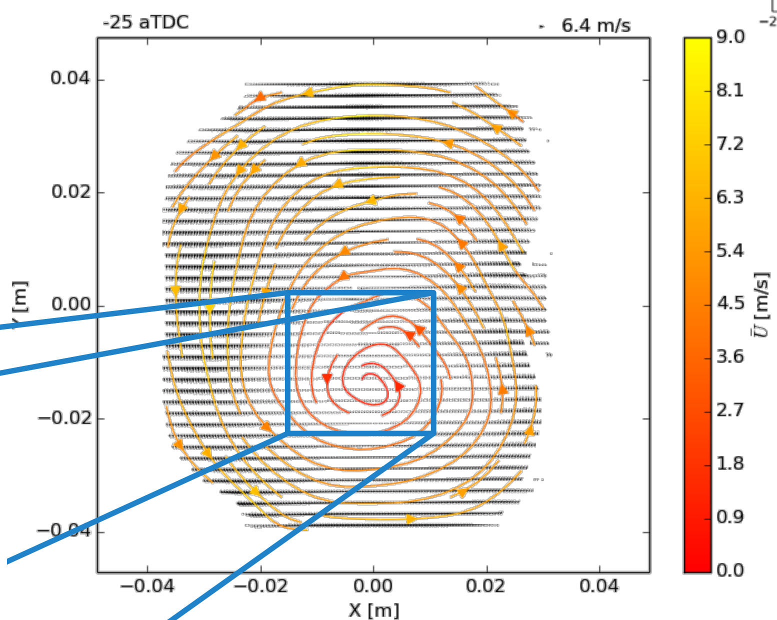
- Flow pattern generally matched.
- Experiments show larger gap in velocity across the spark-plug.
- Pressure well-matched, slightly higher sim peak.

Particle Image Velocimetry



Simulation (PIV Window)





Simulation (Full-Plane)